

EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	173	548/373.1	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/03/08 17:01
L3	255	548/377.1	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/03/08 17:02
L4	2203	514/406	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/03/08 17:03
L5	1	l4 and nr3b1	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT	OR	ON	2007/03/08 17:03

10526940ester

search for when $R_3 = C_1 - C_8$ ^{aminoacyl}
~~amide~~
ester
amide

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 16:38:10 ON 08 MAR 2007

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 16:38:17 ON 08 MAR 2007

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STRUCTURE FILE UPDATES: 7 MAR 2007 HIGHEST RN 925547-09-7

DICTIONARY FILE UPDATES: 7 MAR 2007 HIGHEST RN 925547-09-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
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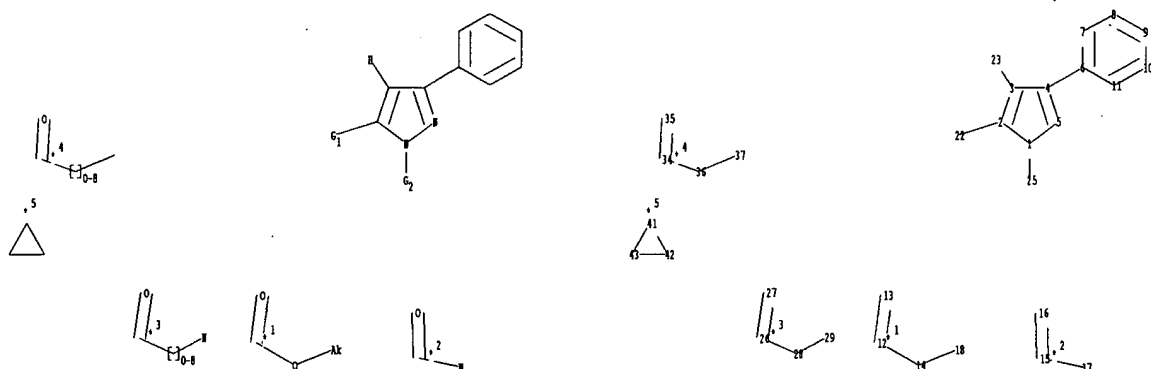
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10526940claim1.str

Karen Cheng



chain nodes :

12 13 14 15 16 17 18 22 23 25 26 27 28 29 34 35 36 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 41 42 43

chain bonds :

1-25 2-22 3-23 4-6 12-13 12-14 14-18 15-16 15-17 26-27 26-28 28-29
34-35 34-36 36-37

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 41-42 41-43 42-43

exact/norm bonds :

1-2 1-5 1-25 2-22 4-5 12-13 12-14 14-18 15-16 15-17 26-27 28-29 34-35

exact bonds :

2-3 3-4 3-23 4-6 26-28 34-36 36-37 41-42 41-43 42-43

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

containing 1 : 6 : 41 :

G1:[*1],[*2],[*3]

G2:H,Ak,[*3],[*4],[*5]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 34:CLASS
35:CLASS 36:CLASS 37:CLASS 41:Atom 42:Atom 43:Atom

10526940ester

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 16:38:36 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 19165 TO ITERATE

100.0% PROCESSED 19165 ITERATIONS
SEARCH TIME: 00.00.01

491 ANSWERS

L2 491 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.10

172.31

FILE 'CAPLUS' ENTERED AT 16:38:40 ON 08 MAR 2007

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FILE COVERS 1907 - 8 Mar 2007 VOL 146 ISS 11

FILE LAST UPDATED: 7 Mar 2007 (20070307/ED)

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=> s l2

L3 87 L2

=> d ibib abs hitstr 50-87

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10526940ester

L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:764057 CAPLUS

DOCUMENT NUMBER: 130:52414

TITLE: Preparation of 3-phenylpyrazole derivatives as

xanthine oxidase inhibitors

INVENTOR(S): Morimoto, Hiroshi; Ishibuchi, Mastake; Fukunari,

Atsushi; Inoue, Hiroyoshi; Naka, Yoichi

PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.

CODEN: JXXXXF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

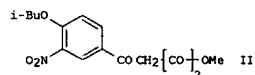
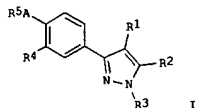
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10310578	A	19981124	JP 1997-307618	19971110
PRIORITY APPLN. INFO.:			JP 1996-301508	A 19961113
			JP 1997-56583	A 19970311

OTHER SOURCE(S): CASREACT 130:52414; MARPAT 130:52414

GI



AB The title compds. (I: R1 = H, halo, OH, NH2, etc.; R2 = CO2H, alkoxycarbonyl, HOCH2, etc.; R3 = H, alkyl, haloalkyl, etc.; R4 = NO2, CN, acyl, etc.; R5 = H, alkyl, haloalkyl, cycloalkyl, etc.; A = O, S, SO, SO2) are prepared I, possessing xanthine oxidase receptor inhibitory activity (IC50 < 30 nM), are useful for the treatment and prevention of high urine acidosis and as uric acid excretory agents. Thus, compound (II) was refluxed with NH2NH2 in EtOH for 30 min to give I (R1 = R3 = H, R2 = CO2Me, R4 = NO2, R5 = iso-Bu, A = O). A formulation containing I was also prepared

IT 217484-33-8P 217484-35-0P, 217484-37-2P

L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

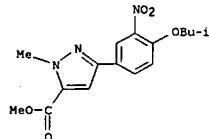
217484-39-4P 217484-43-0P 217484-45-2P
 217484-47-4P 217484-49-6P 217484-51-0P
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 217484-65-6P 217484-67-8P 217484-69-0P
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 217484-77-0P 217484-79-2P 217484-81-6P
 217484-83-8P 217484-84-9P 217484-85-0P
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 217484-93-0P 217484-95-2P 217484-97-4P
 217484-99-6P 217485-01-3P 217485-03-5P
 217485-05-7P 217485-07-9P 217485-09-1P
 217485-11-5P 217485-13-7P 217485-16-0P
 217485-20-6P 217485-26-2P 217485-32-0P
 217485-34-2P 217485-36-4P 217485-42-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-phenylpyrazole derivs. as xanthine oxidase inhibitors)

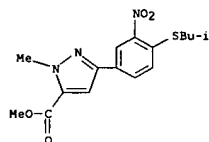
RN 217484-33-8 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-3-[4-(2-methylpropoxy)-3-nitrophenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 217484-35-0 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-3-[4-[(2-methylpropyl)thio]-3-nitrophenyl]-, methyl ester (9CI) (CA INDEX NAME)

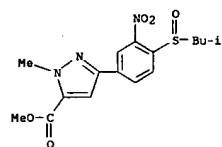


RN 217484-37-2 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-3-[4-(2-methylpropyl)sulfinyl]-3-

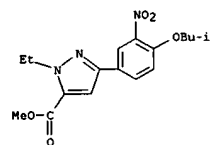
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

nitrophenyl]-, methyl ester (9CI) (CA INDEX NAME)



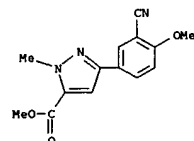
RN 217484-39-4 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 1-ethyl-3-[4-(2-methylpropoxy)-3-nitrophenyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 217484-43-0 CAPLUS

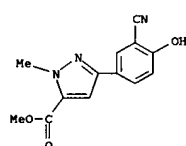
CN 1H-Pyrazole-5-carboxylic acid, 3-(3-cyano-4-methoxyphenyl)-1-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 217484-45-2 CAPLUS

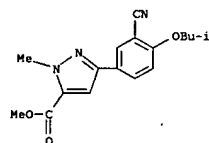
CN 1H-Pyrazole-5-carboxylic acid, 3-(3-cyano-4-hydroxyphenyl)-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



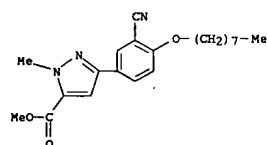
RN 217484-47-4 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2-methylpropoxy)phenyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 217484-49-6 CAPLUS

CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(octyloxy)phenyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

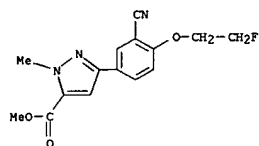


RN 217484-51-0 CAPLUS

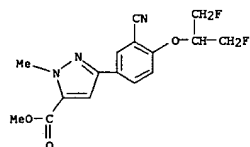
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2-fluoroethoxy)phenyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

10526940ester

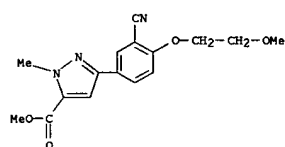
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-53-2 CAPLUS
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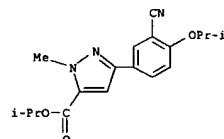


RN 217484-55-4 CAPLUS
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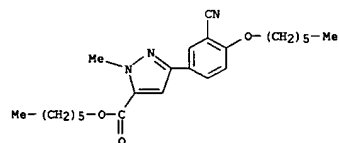


RN 217484-57-6 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(cyclopropylmethoxy)phenyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

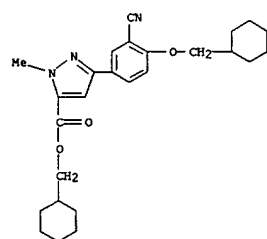
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-65-6 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(hexyloxy)phenyl]-1-methyl-, hexyl ester (9CI) (CA INDEX NAME)

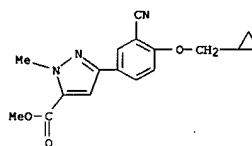


RN 217484-67-8 CAPLUS
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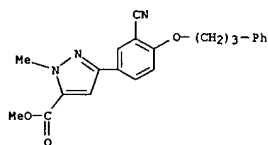


RN 217484-69-0 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(propoxyphenyl)-1-methyl-, propyl ester (9CI) (CA INDEX NAME)

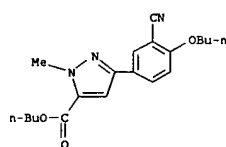
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-59-8 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(3-phenylpropoxy)phenyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)

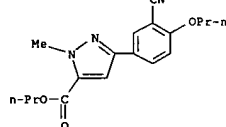


RN 217484-61-2 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-(4-butoxy-3-cyanophenyl)-1-methyl-, butyl ester (9CI) (CA INDEX NAME)

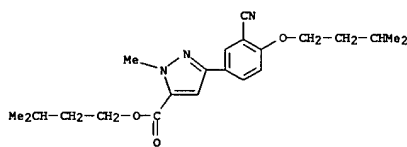


RN 217484-63-4 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(1-methylethoxy)phenyl]-1-methyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)

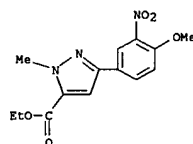
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-71-4 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(3-methylbutoxy)phenyl]-1-methyl-, 3-methylbutyl ester (9CI) (CA INDEX NAME)



RN 217484-73-6 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-(4-methoxy-3-nitrophenyl)-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

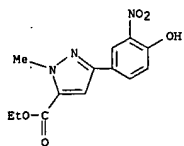


RN 217484-75-8 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-(4-hydroxy-3-nitrophenyl)-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

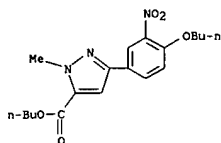
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10526940ester

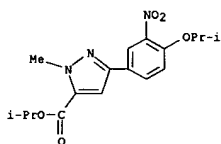
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-77-0 CAPLUS
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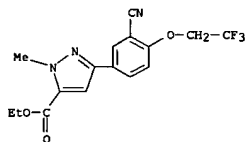


RN 217484-79-2 CAPLUS
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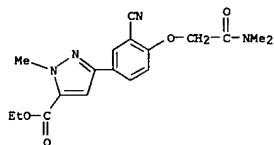


RN 217484-81-6 CAPLUS
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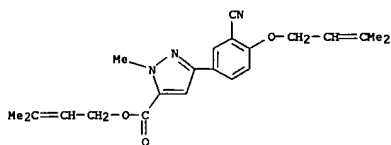
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-87-2 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-[2-(dimethylamino)-2-oxoethoxy]phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

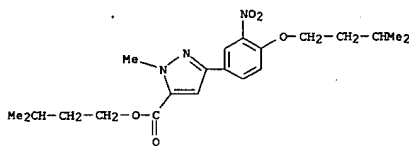


RN 217484-89-4 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-[(3-methyl-2-butenyl)oxy]phenyl]-1-methyl-, 3-methyl-2-butenyl ester (9CI) (CA INDEX NAME)

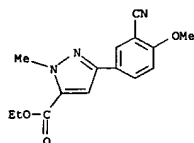


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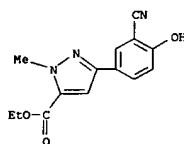
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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CN 1H-Pyrazole-5-carboxylic acid, 3-(3-cyano-4-methoxyphenyl)-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

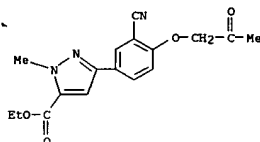


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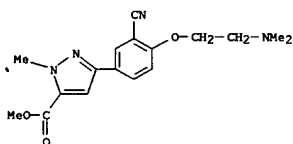


RN 217484-85-0 CAPLUS
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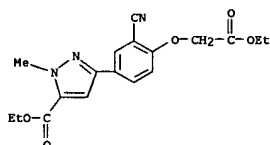
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-93-0 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-[2-(dimethylamino)ethoxy]phenyl]-1-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 217484-95-2 CAPLUS
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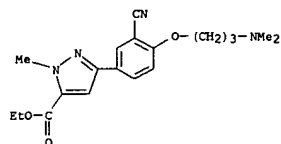


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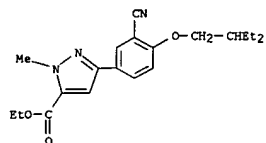
Karen Cheng

10526940ester

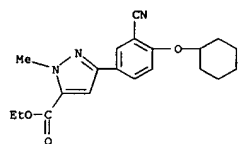
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217484-99-6 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2-ethylbutoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

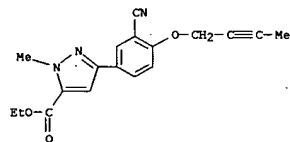


RN 217485-01-3 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(cyclohexyloxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

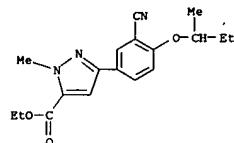


RN 217485-03-5 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(1-ethylpropoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

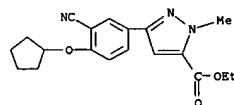
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217485-11-5 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(1-methylpropoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

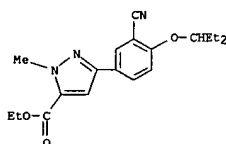


RN 217485-13-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(cyclopentyloxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

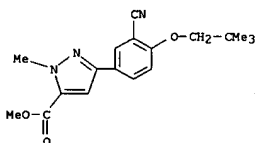


RN 217485-16-0 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2-methylbutoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

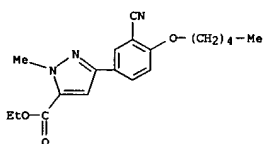
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217485-05-7 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2,2-dimethylpropoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

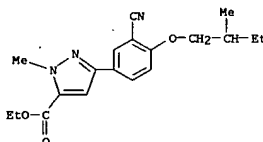


RN 217485-07-9 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(pentyloxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

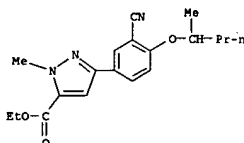


RN 217485-09-1 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[4-(2-butynyloxy)-3-cyanophenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

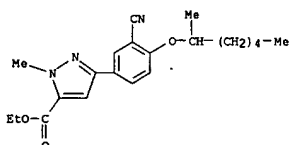
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217485-20-6 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(1-methylbutoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)



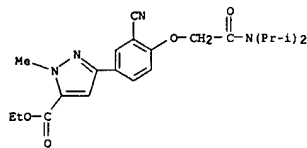
RN 217485-26-2 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-[(1-methylhexyl)oxy]phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)



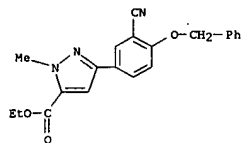
RN 217485-32-0 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[4-[2-bis(1-methylethyl)amino]-2-oxoethoxy]-3-cyanophenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)

10526940ester

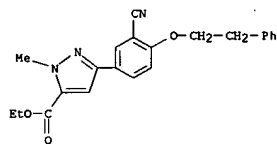
L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 217485-34-2 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(phenylmethoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 217485-36-4 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2-phenylethoxy)phenyl]-1-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 217485-42-2 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 3-[3-cyano-4-(2-methylpropoxy)phenyl]-1-methyl-, 2-(dimethylamino)-2-oxoethyl ester (9CI) (CA INDEX NAME)

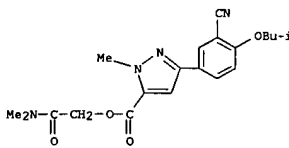
L3 ANSWER 51 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:717885 CAPLUS
DOCUMENT NUMBER: 127:331484
TITLE: Preparation of ethylene derivatives as pest controlling agents
INVENTOR(S): Ogura, Tomoyuki; Murakami, Hiroshi; Numata, Akira; Miyachi, Rika
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan; Ogura, Tomoyuki;
SOURCE: PCT Int. Appl., 423 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

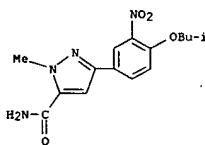
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9740009	A1	19971030	WO 1997-JP1440	19970424
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LX, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, HL, HR, NE, SN, TD, TG				
CA 2252536	A1	19971030	CA 1997-2252536	19970424
JP 9724071	A	19971112	AU 1997-24071	19970424
AU 736854	B2	20010802		
ZA 9703563	A	19980115	ZA 1997-3563	19970424
EP 913392	A1	19990506	EP 1997-919686	19970424
EP 913392	B1	20030702		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1216530	A	19990512	CN 1997-194041	19970424
BR 9709126	A	20000111	BR 1997-9126	19970424
TW 449460	B	20010811	TW 1997-86105307	19970424
AT 244219	T	20030715	AT 1997-919686	19970424
EP 1360901	A1	20031112	EP 2003-9790	19970424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PT 913392	T	20031128	PT 1997-919686	19970424
JP 2003342262	A	20031203	JP 2003-109445	19970424
ES 2201293	T3	20040316	ES 1997-919686	19970424
CN 1763003	A	20060426	CN 2005-10116118	19970424
US 6063734	A	20000516	US 1998-177501	19981023
KR 2000010635	A	20000225	KR 1998-708544	19981024
US 6462049	B1	20021008	US 2000-492321	20000127
US 38188	E1	20030715	US 2001-983477	20011024
US 2003216394	A1	20031120	US 2002-214258	20020808
US 7037880	B2	20060502		
US 2007049495	A1	20070301	US 2005-203341	20050815
PRIORITY APPLN. INFO.:				
			JP 1996-104878	A 19960425
			JP 1996-145802	A 19960607
			JP 1996-159346	A 19960620
			JP 1997-28916	A 19970213
			CN 1997-194041	A3 19970424
			EP 1997-919686	A3 19970424
			JP 1997-537934	A3 19970424
			WO 1997-JP1440	W 19970424

Karen Cheng

L3 ANSWER 50 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

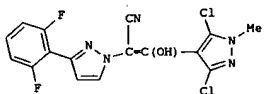


IT 217485-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-phenylpyrazole derivs. as xanthine oxidase inhibitors)
RN 217485-60-4 CAPLUS
CN 1H-Pyrazole-5-carboxamide, 1-methyl-3-[4-(2-methylpropoxy)-3-nitrophenyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 51 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 1998-177501 A3 19981023
US 2000-492321 A3 20000127
US 2002-214258 A1 20020808
OTHER SOURCE(S): MARPAT 127:331484
GI

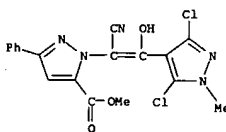


AB Phenylheterocyclylethylene derivs. of general formula EC(Q):C(A)OB(A, Q = (un)substituted Ph, naphthyl, or heterocyclyl, particularly, 4-thiazolyl, 1- or 3-pyrazolyl, 1,3-oxazol-4-yl, Ph, or pyridyl; E = cyano, or the like; A is 4-pyrazolyl, thiazolyl or the like; B = H, Cl-4 (halo)alkyl, C2-4 alkoxyalkyl, MeSCH2, MeOCH2CH2OCH2, (un)substituted phenyl-C1-4 alkyl or benzoyl-C1-4 alkyl, tetrahydropyranyl, Me3Si, Cl-4 alkylsulfonyl, etc.; E = optionally Cl-4 alkyl or Cl-4 haloalkyl-substituted heterocyclyl, C2-4 alkynyl, (un)substituted phenylethynyl, Cl-4 haloalkyl, cyano, NO2, N3, CHO, (un)substituted COPH, etc.), which are useful as insecticides, aphicides, acaricides, and fungicides, are prepared. Pesticides or aquatic organism adhesion inhibitors containing at least one of the above derivs.

are claimed. Thus, 1-cyanomethyl-3-(2,6-difluorophenyl)pyrazole was stirred with NaH in THF at 50° for 30 min, followed by adding dropwise a solution of 1-(1-methyl-3,5-dichloropyrazole-4-carbonyl)pyrazole in THF at 50°, and the resulting mixture was stirred at room temperature overnight to give the title compound (I). I at 500 ppm controlled 280U organophosphorus-resistant Nephrotettix cincticeps, Myzus persicae, larvae of Plutella xylostella Plutella xylostella konaga, and Tetranychus urticae.

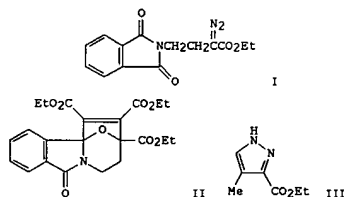
IT 198070-96-1P 198070-97-2P 198070-98-3P
198071-00-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of ethylene derivs. as pesticides)

RN 198070-96-1 CAPLUS
CN 1H-Pyrazole-5-carboxylic acid, 1-[1-cyano-2-(3,5-dichloro-1-methyl-1H-pyrazol-4-yl)-2-hydroxyethenyl]-3-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 63 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

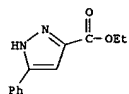
L3 ANSWER 64 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1990:423815 CAPLUS
 DOCUMENT NUMBER: 113:23815
 TITLE: Reaction of carbonyl compounds with ethyl lithiodiazoacetate. Studies dealing with the rhodium(II)-catalyzed behavior of the resulting adducts
 AUTHOR(S): Padwa, Albert; Kulkarni, Yashwant S.; Zhang, Zhijia
 CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
 SOURCE: Journal of Organic Chemistry (1990), 55(13), 4144-53
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 113:23815
 GI



AB The carbenoid intermediate derived by treating Et 2-diazo-4-phthalimidovalerate (I) with rhodium(II) octanoate undergoes transannular cyclization onto the adjacent imido carbonyl group. The resulting cyclic carbonyl ylide dipole reacted with dipolarophiles to give adducts, e.g. II. The reaction of Et lithiodiazoacetate with various aldehydes and ketones was also studied. Treatment of α -diazo- β -hydroxy esters, e.g. $\text{HOCH}_2\text{C}(\text{CO}_2\text{Et})\text{:N}_2$, derived from Me_2CO or cyclopentanone with rhodium(II) octanoate gave rise to β -keto esters, e.g. $\text{MeCOCH}_2\text{CO}_2\text{Et}$. The exclusive Ph shift encountered with PhOCMe is in keeping with migration to an electron-deficient center. The reaction works well with $\text{H}_2\text{C:CHCO}_2\text{H}$, leading to high yields of $\text{H}_2\text{C:CHCOCH}_2\text{CO}_2\text{Et}$. The 1,2-hydrogen shift pathway was found to proceed much faster than intramolecular cyclopropanation. Dehydration of the α -diazo- β -hydroxy esters generates vinyl diazo esters, e.g. $\text{H}_2\text{C:CMeC}(\text{CO}_2\text{Et})\text{:N}_2$, which readily cyclizes to 1H-pyrazoles, e.g. III, on thermolysis.

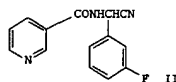
IT 5932-30-9P
 RI: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 5932-30-9 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 5-phenyl-, ethyl ester (9CI) (CA INDEX)

L3 ANSWER 64 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L3 ANSWER 65 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1989:75498 CAPLUS
 DOCUMENT NUMBER: 110:75498
 TITLE: Preparation of heterocyclamidooxonitriles as agrochemical microbicides
 INVENTOR(S): Suzuki, Hideo; Mita, Takeshi; Fukuda, Kenzo; Ochiai, Yoshinori; Hanaue, Masami; Nishikubo, Masao
 PATENT ASSIGNER(S): Nissan Chemical Industries, Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
 CODEN: JNOXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63135364	A	19880607	JP 1986-283881	19861128
PRIORITY APPLN. INFO.:			JP 1986-283881	19861128
OTHER SOURCE(S):			CASREACT 110:75498; MARPAT 110:75498	
GI				

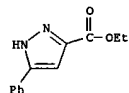


AB Title compds. ACONR1CR2R3CN [I; A = heterocyclyl (a number of structures are given, e.g. pyridyl, benzopyrazolyl; dihydropyranyl, and dioxothiophenyl); R1, R2 = H, alkyl; R3 = (substituted) cyclohexyl, (substituted) Ph, (substituted) naphthalen-1- and -2-yl, (substituted) 1,2,3,4-tetrahydronaphthalen-5- and -6-yl] are prepared by Strecker synthesis of R2R3CO with R1NH2 in the presence of KCN, followed by amidation of the resulting R1NHCR2R3CN with ACOCN. To a mixture of NH_4Cl , KCN, and 28% aqueous NH_3 was added a solution of $m\text{-FC}_6\text{H}_4\text{CHO}$ in PhMe at 0° . stirring the resultant mixture at room temperature overnight gave 82.0% $m\text{-FC}_6\text{H}_4(\text{H}_2\text{N})\text{CHCN}$, which was treated with nicotinic acid chloride HCl in MeCN in the presence of Et3N at 0° to room temperature to afford 77.7% a nicotinamide II, which at 500 ppm showed 100% control of Pseudoperonospora cubensis and a minor damage on cucumbers, vs. 65% for zineb. A wettable powder was formulated containing I 25, zeeklite 69, sorpol 5039 3, and carplex 3 weight parts.

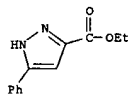
IT 118880-74-3P
 RI: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as agrochem. microbicide)
 RN 118880-74-3 CAPLUS
 CN 1H-Pyrazole-5-carboxamide, 3-(4-chlorophenyl)-N-(cyanophenylmethyl)-1-methyl- (9CI) (CA INDEX NAME)

10526940ester

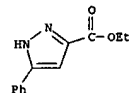
L3 ANSWER 78 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1967:80664 CAPLUS
 DOCUMENT NUMBER: 66:80664
 TITLE: Azoles. XIV. Ultraviolet study of pyrazoles
 AUTHOR(S): Elguero, Jose; Jacquier, Robert; Nguyen Tien Duc Hong
 CORPORATE SOURCE: Fac. Sci., E.N.S.C.M., Montpellier, Fr.
 SOURCE: Bulletin de la Societe Chimique de France (1966), (12), 3744-52
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI For diagram(s), see printed CA Issue.
 AB cf. preceding abstract The uv spectra of 170 NH and N-substituted pyrazoles of general structure I were determined at 95° in EtOH. Some of the substituents were Me, CONH2, Ac, p-MeC6H4SO2, Ph, p-BrC6H4, p-O2NC6H4, 2,4-(O2N)2C6H3, and 2,4,6-(O2N)3C6H2. In the 2,4-(O2N)2C6H3 and 2,4,6-(O2N)3C6H2 series a time dependence of spectra is noted. Uv spectra are able to identify pairs of N-substituted pyrazole isomers.
 IT 5932-30-9
 RL: PRP (Properties) (spectrum (visible and uv) of)
 RN 5932-30-9 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



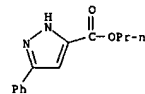
L3 ANSWER 79 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1967:80663 CAPLUS
 DOCUMENT NUMBER: 66:80663
 TITLE: Azoles. XIII. Nuclear magnetic resonance spectra of pyrazoles
 AUTHOR(S): Elguero, Jose; Jacquier, Robert; Nguyen Tien Duc Hong
 CORPORATE SOURCE: Fac. Sci., E.N.S.C.M., Montpellier, Fr.
 SOURCE: Bulletin de la Societe Chimique de France (1966), (12), 3727-43
 CODEN: BSCFAS; ISSN: 0037-8968
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 AB cf. preceding abstract The N.M.R. spectra of 180 pyrazoles in nonaq. solvents (CDCl3, CCl4, C6H6, Me2SO, CF3CO2H) were analyzed. Classes represented were non-N-substituted, N-alkyl (especially N-Me), N-carboxamide, N-tosyl, N-Ph, N-p-nitrophenyl, N-(2,4-dinitrophenyl), and 2,4,6-trinitrophenyl pyrazoles. Chemical displacements (τ) and coupling consts. (J) were calculated and compared with literature values.
 Differences in values were attributed to substituents in ring positions 3, 4, and 5. Steric hindrance between the pyrazolic nucleus and aromatic substituents and the effect of C-Me groups on shielding of the pyrazolic protons was studied. 85 references.
 IT 5932-30-9
 RL: PRP (Properties) (N.M.R. of)
 RN 5932-30-9 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 80 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1967:75947 CAPLUS
 DOCUMENT NUMBER: 66:75947
 TITLE: Esters of oxo acids of acetylene series. VI. Reaction of the esters of phenylethynylglyoxalic acid with hydrazine, hydrazide, and hydroxylamine
 AUTHOR(S): Lapkin, I. I.; Andreichikov, Yu. S.
 SOURCE: Zhurnal Organicheskoi Khimii (1966), 2(11), 2075-8
 CODEN: ZORKAE; ISSN: 0514-7492
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 OTHER SOURCE(S): CASREACT 66:75947
 AB cf. CA 65, 10523b. Addition of N2H4.H2O to Et phenylethynylglyoxalate in EtOH gave 75% Et 3-phenylpyrazole-5-carboxylate, m. 139.5°; similarly were prepared: Pr ester, m. 110°; iso-Pr ester, m. 164°. Addition of RHNH2 in Et2O to the appropriate ester of phenylethynylglyoxalic acid gave the following esters of 4-arylhydrazino-4-phenyl-3-buten-2-on-1-ic acids, RHNHCFPh:CCOCO2R (R and R' shown, resp.): Ph, Et, 32%, m. 83°; Ph, iso-Pr (I) 65%, m. 124.5°; p-MeC6H4, iso-Pr, 32%, m. 77°; O-MeC6H4, iso-Pr, 55%, m. 72.5°; Bz, iso-Pr (II) 87%, m. 125.5°; O-O2NC6H4CO, iso-Pr, 78%, m. 137°; m-O2NC6H4CO, iso-Pr, 83%, m. 181°; p-O2NC6H4CO, iso-Pr, 88%, m. 175°. II heated in AcOH 2 hrs. gave 93% 1,5-diphenylpyrazole-3-carboxylic acid iso-Pr ester, m. 86.5-7°. I heated with aqueous alc. KOH 20 min. gave 1,5-diphenylpyrazole-3-carboxylic acid. Heating iso-Pr phenylethynylglyoxalate with HONH2.HCl in aqueous EtOH gave after addition of aqueous Na2CO3 over 9 hrs. 50% iso-Pr 3-phenylisoxazole-5-carboxylate, m. 65-6°. Similarly was prepared 29% Et 3-phenylisoxazole-5-carboxylate, m. 47°. Ir spectra were reported.
 IT 5932-30-9P 13599-13-8P 13599-14-9P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)
 RN 5932-30-9 CAPLUS
 CN 1H-Pyrazole-3-carboxylic acid, 5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

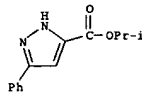


RN 13599-13-8 CAPLUS
 CN Pyrazole-3-carboxylic acid, 5-phenyl-, propyl ester (8CI) (CA INDEX NAME)



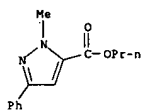
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L3 ANSWER 80 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 RN 13599-14-9 CAPLUS
 CN Pyrazole-3-carboxylic acid, 5-phenyl-, isopropyl ester (8CI) (CA INDEX NAME)



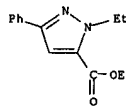
10526940ester

L3 ANSWER 81 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1966:420199 CAPLUS
 DOCUMENT NUMBER: 65:20199
 ORIGINAL REFERENCE NO.: 65:3707c-e
 TITLE: Proton magnetic resonance studies of pyrazoles
 AUTHOR(S): Tensmeyer, L. G.; Ainsworth, C.
 CORPORATE SOURCE: Lilly Res. Labs., Indianapolis, IN
 SOURCE: Journal of Organic Chemistry (1966), 31(6), 1878-83
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB 4-Proton chemical shift data for 54 pyrazoles are correlated in the empirical equation $\delta_4 = \delta_4(s) + a_1 + a_3 + a_5$, where $\delta_4(s)$ is a constant for each solvent, and a_1 , a_3 , and a_5 are empirical consts. that represent the effect of replacing a methyl substituent by another group at positions 1, 3, and 5 of the pyrazole nucleus. The equation can be used for isomer identification and for the study of tautomers. The a consts. of the equation are correlated with Hammett σ consts. In the N.M.R. spectra, a phenyl group attached to a pyrazole ring appears as a multiplet resonance unless a substituent is α to it. Under the latter condition the phenyl resonance is a singlet. Chemical shift data are used to distinguish relative coplanarity of the phenyl and pyrazole rings. Ring proton coupling consts. of pyrazoles are discussed.
 IT 10199-49-2, Pyrazole-5-carboxylic acid, 1-methyl-3-phenyl-, propyl ester 10199-55-0, Pyrazole-5-carboxylic acid, 1-ethyl-3-phenyl-, ethyl ester 10250-62-1, Pyrazole-5-carboxylic acid, 1-methyl-3-phenyl-, methyl ester 10250-63-2, Pyrazole-5-carboxylic acid, 1-methyl-3-phenyl-, ethyl ester (nuclear magnetic resonance of)
 RN 10199-49-2 CAPLUS
 CN Pyrazole-5-carboxylic acid, 1-methyl-3-phenyl-, propyl ester (7CI, 8CI) (CA INDEX NAME)

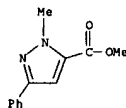


RN 10199-55-0 CAPLUS
 CN 1H-Pyrazole-1-carboxylic acid, 1-ethyl-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

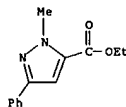
L3 ANSWER 81 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 10250-62-1 CAPLUS
 CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-3-phenyl-, methyl ester (9CI) (CA INDEX NAME)



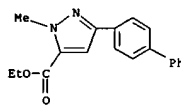
RN 10250-63-2 CAPLUS
 CN 1H-Pyrazole-5-carboxylic acid, 1-methyl-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 82 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1959:105517 CAPLUS
 DOCUMENT NUMBER: 53:105517
 ORIGINAL REFERENCE NO.: 53:189421, 18943a-g
 TITLE: Ethyl p-phenylbenzoylpyruvate and its cyclization products
 AUTHOR(S): Fatutta, Silvana; Balestra, Mario
 CORPORATE SOURCE: Univ. Trieste
 SOURCE: Gazzetta Chimica Italiana (1958), 88, 899-909
 CODEN: GCITA9; ISSN: 0016-5603
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. C.A. 51, 15517d. (CO₂Et)₂ (6.7 g.) and 9.8 g. p-PhCGH₄COMe in 500 ml. perfectly dry Et₂O stirred 4-5 hrs. at 0° with 1.1 g. finely divided Na, the mixture refluxed on a steam bath 8 hrs. with constant stirring and the cooled mixture filtered, the Na salt washed repeatedly with dry Et₂O and anhydrous alc. to remove all traces of p-PhCGH₄COMe and the salt suspended in H₂O, the suspension stirred vigorously with addition of dilute AcOH and the acidified mixture filtered gave the title compound (I), m. 114° (95% alc.); Cu(II) compound, C₃H₃OCuO₈; Fe(III) compound, C₅H₄FeO₁₂. I (2 g.) in a min. of alc. and 0.700 g. N₂H₄.HCl in a min. of H₂O heated 4 hrs. on a steam bath and the cooled mixture kept several hrs., filtered and the brown precipitate washed with alc. gave Et 5-(p-biphenyl)-3-pyrazolecarboxylate (II), m. 191° (alc.), hydrolyzed by refluxing 6 hrs. with 50% alc. KOH and evaporating the excess alc., taking up in H₂O and acidifying with dilute HCl to give the corresponding acid, m. 281° (alc.). I (1 g.) in a min. of alc. refluxed 4 hrs. with 0.400 g. PhNHNH₂.HCl in H₂O and the product crystallized (alc.) gave the Et ester, m. 126°, hydrolyzed with 50% KOH as above to give the corresponding 5-(p-biphenyl)-1-phenyl-3-pyrazolecarboxylic acid (III), m. 208°. III (0.200 g.) heated 2 hrs. (oil bath) at 235° and the cooled product digested with aqueous NaHCO₃, washed with H₂O and crystallized (95% alc.) gave 5-(p-biphenyl)-1-phenylpyrazole, m. 138°. I (0.200 g.) in 13 ml. AcOH refluxed 10 min. with 0.5 ml. MeNHNH₂ and the cooled product diluted with H₂O, the mixture extracted with Et₂O and the extract evaporated gave Et 5-(p-biphenyl)-1-methyl-3-pyrazolecarboxylate, m. 108°. II (0.200 g.) kept 24 hrs. with excess CH₂N₂ in Et₂O and the excess Et₂O evaporated gave Et 3-(p-biphenyl)-1-methyl-5-pyrazolecarboxylate, m. 93°. I (0.700 g.) in 50 ml. alc. heated on a steam bath 4 hrs. with 0.500 g. HONH₂.HCl in a min. of H₂O and the cooled solution filtered gave Et 4-(p-biphenyl)-3-isoxazolecarboxylate, saponified by refluxing 2 hrs. in alc. KOH and concentrating, diluting with H₂O and acidifying to give the corresponding acid (IV), m. 210° (alc.). IV (1 g.) heated (oil bath) 30 min. at 215° with evolution of CO₂ and the cooled product taken up in AcOH, the filtered solution kept 5 hrs. with p-O₂NC₆H₄NHNH₂ in AcOH and the mixture heated 1 hr. on a steam bath, the cooled mixture diluted with distilled H₂O and filtered gave brick-red 3-amino-5-(p-biphenyl)-2-(p-nitrophenyl)pyrazole, m. 216°, diazotized and coupled with β-C₁₀H₇OH to give a dark red azo dye. I (0.200 g.) and 0.100 g. NCH₂CONH₂ in a min. of alc. and 0.1 ml. anhydrous HNEt₂ kept 24 hrs. at room temperature and the solvent evaporated spontaneously at room temperature gave

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L3 ANSWER 82 OF 87 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
 6-(p-biphenyl)-4-carbomethoxy-3-cyano-2(1H)-pyridone (VI), m. 272° (alc.). V (0.200 g.) kept 24 hrs. with excess CH₂N₂ in Et₂O and the insol. product crystd. (alc.) gave 6-(p-biphenyl)-4-carbomethoxy-3-cyano-1-methyl-2(1H)-pyridone (VI), m. 207°. The filtrate from VI evapd. and the residue crystd. (alc.) gave 6-(p-biphenyl)-4-carbomethoxy-3-cyano-2-methoxypyridine, m. 155°. I (0.300 g.) and 0.100 g. NCH₂CONH₂ in a min. of alc. kept 24 hrs. with 0.2 ml. HNEt₂, the alc. evapd. at room temp. and the residue crystd. (alc.) gave authentic VI.
 IT 110145-11-4P, Pyrazole-5-carboxylic acid, 3-(4-biphenyl)-1-methyl-, ethyl ester
 RL: PREP (Preparation)
 (preparation of)
 RN 110145-11-4 CAPLUS
 CN Pyrazole-5-carboxylic acid, 3-(4-biphenyl)-1-methyl-, ethyl ester (6CI) (CA INDEX NAME)



10526940species

Search for deleted species

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AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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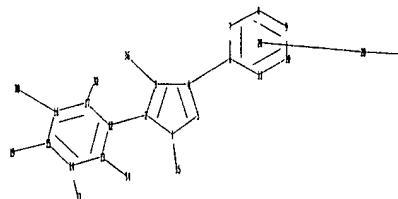
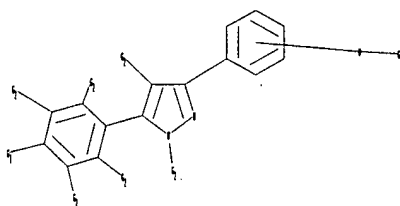
<http://www.cas.org/ONLINE/UG/regprops.html>

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chain nodes :
19 20 21 22 23 24 27 30 32 33 34 35 36
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
chain bonds :
1-35 2-12 3-36 4-6 13-34 14-33 15-19 16-30 17-32 20-27 21-22 21-23
21-24
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14
14-15 15-16 16-17
exact/norm bonds :
1-2 1-5 1-35 3-36 4-5 13-34 14-33 15-19 16-30 17-32 20-27
exact bonds :
2-3 2-12 3-4 4-6 21-22 21-23 21-24
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17
isolated ring systems :
containing 1 : 6 : 12 :

G1:Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G2:H, [*1]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 27:CLASS 28:Atom 30:CLASS 32:CLASS
33:CLASS 34:CLASS 35:CLASS 36:CLASS

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L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR

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FULL SCREEN SEARCH COMPLETED - 36734 TO ITERATE

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SEARCH TIME: 00.00.01

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SINCE FILE

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ENTRY

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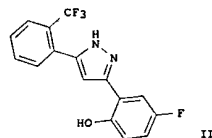
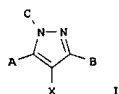
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10526940species

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:780671 CAPLUS
DOCUMENT NUMBER: 141:296010
TITLE: Preparation of substituted pyrazoles as modulators of
ATP-binding cassette transporters
INVENTOR(S): Vangoor, Frederick F.; Hadida Ruah, Sarah S.; Singh,
Ashvani K.; Olson, Eric R.; Makings, Lewis R.;
Gonzalez, Jesus E., III; Rader, James A.; Chambers,
Fred, III; Miller, Mark T.; Grootenhuis, Peter; Liu,
Yahua
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 174 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080972	A1	20040923	WO 2004-US7492	20040312
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2005113423	A1	20050526	US 2004-800022	20040312
EP 1601657	A1	20051207	EP 2004-720345	20040312
R:	AE, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK			
PRIORITY APPL. INFO.:			US 2003-453978P	P 20030312
			WO 2004-US7492	W 20040312

OTHER SOURCE(S): MARPAT 141:296010
GI

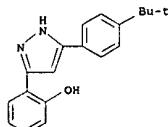


L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Pyrazoles I [A, B = (un)substituted aryl, heterocyclyl, cycloalkyl; C = H, (un)substituted aryl, heterocyclyl, heteroaryl, cycloalkyl, alkyl, alkylcarbonyl, arylcarbonyl, heteroarylcarbonyl, heterocyclylcarbonyl, or aminocarbonyl; X = H, (un)substituted alkyl, aryl, heterocyclyl, heteroaryl, or n-substituted n-alkyl] such as II are prepared as inhibitors of ATP-binding cassette (ABC) transporters such as the cystic fibrosis transmembrane conductance regulator (CFTR) for use in the treatment of conditions such as cystic fibrosis, immunodeficiency, inflammatory disease, chronic obstructive pulmonary disease, chronic pancreatitis, or pneumonia. 4-Trifluoromethylbenzoyl chloride and 2-hydroxy-5-fluoroacetophenone are stirred in pyridine for 12 h, after which potassium hydroxide is added and the mixture stirred for 12 h; addition of hydrazine hydrate to a solution of the product obtained in the first step in ethanol and heating at reflux for 3 h yields II in 30% overall yield as a yellow crystalline solid. II modulates $\Delta F508$ -CFTR at 275% of the effect of genistein on the same receptor. Data on the relative modulation of $\Delta F508$ -CFTR by some compds. of the invention as compared to genistein is provided.

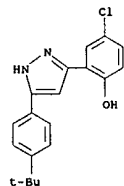
IT 423750-83-8P 423752-83-4P
RL: PAC (Pharmacological activity); SPM (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazoles as modulators of ATP-binding cassette transporters such as the cystic fibrosis transmembrane conductance regulator for treatment of diseases such as cystic fibrosis, immunodeficiency, and pneumonia)

RN 423750-83-8 CAPLUS
CN Phenol, 2-[5-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



RN 423752-83-4 CAPLUS
CN Phenol, 4-chloro-2-[5-[4-(1,1-dimethylethyl)phenyl]-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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